PHYS 6350 HW8. Due Friday Dec 4 at 9am

1. **6 pts** Write a program that generates a random number in the interval $[1, T)$ for some T, with probablity $p(x) \propto x^{-1}$. For $T = 10$, generate 10^5 numbers using this program, and plot the distribution.

2. **14 points** N identical particles in three dimensions are harmonically bound to the origin, with $V_{ext} = \frac{k_1}{2}\sum_j \mathbf{r}_j^2$. They interact with each other with a central force potential $V_{int}(|\mathbf{r}_1 - \mathbf{r}_2|)$. The Langevin equation for each particle is $m\ddot{\mathbf{r}}_i = -\zeta\dot{\mathbf{r}}_i - \nabla_i[V_{ext}(\mathbf{r}_i) + \sum_j V_{int}(|\mathbf{r}_i - \mathbf{r}_j)|]) + \mathbf{F}_i$, where each component of all random forces are uncorrelated with zero mean: $\langle(\mathbf{F}_i(t))_j\rangle = 0$ and $\langle(\mathbf{F}_i(t))_j(\mathbf{F}_k(t))_l = 2\zeta k_B T\delta_{ik}\delta_{jl}\delta(t - t')$.

   (a) Show that the center of mass of the particles, $\mathbf{R} = N^{-1}\sum_i \mathbf{r}_i$, evolves under the effective Langevin equation $m\ddot{\mathbf{R}} = -\zeta\dot{\mathbf{R}} - k_1\mathbf{R} + \mathbf{F}_c$, with an effective random force satisfying $\langle\mathbf{F}_c\rangle = 0$ and $\langle(\mathbf{F}_c(t))_i(\mathbf{F}_c(t))_j\rangle = 2\zeta k_B T/N\delta_{ij}$.

   (b) Solve the effective Langevin equation in (a), to show that if the initial conditions are $\mathbf{R}(0) = 0$ and $\dot{\mathbf{R}}(0) = 0$, that

   $$\mathbf{R}(t) = \int_0^t dt' \frac{2\tau_2}{m} e^{-(t-t')/2\tau_1} \sinh\left(\frac{t - t'}{2\tau_2}\right)\mathbf{F}_c(t') \tag{1}$$

   Use this to determine $\langle\mathbf{R}^2(t)\rangle$. *Hint* To find $\mathbf{R}(t)$, using a Laplace Transform and the convolution theorems are likely to be helpful. Using eq. (1), the calculation of $\langle\mathbf{R}^2(t)\rangle$ does not require any special tricks (but is tedious to calculate).

   (c) Using the nondimensional units $m = \zeta = k_B T = 1$, and with $k_1 = 0.1$ in those units, simulate the dynamics of $N = 2$ particles with a harmonic bond between them, $V_{int}(x) = k_2(x - a)^2/2$, with $k_2 = a = 1$ in the dimensionless units. Perform 1,000 simulations starting from the initial conditions $\mathbf{r}_1(0) = (-0.5, 0, 0)$ and $\mathbf{r}_2(0) = (0.5, 0, 0)$, and with $\dot{\mathbf{r}}_i(0) = 0$ for all particles. Compute $\langle\mathbf{v}^2(t)\rangle$ (with the average taken over your 1000 simulations), and determine if your simulation agrees with the equipartition of energy. Also plot $\langle\mathbf{R}^2\rangle$ and compare to your theoretical prediction in (b).